

IN THE SPECIFICATION:

Please amend the paragraph beginning at page 8, line 6 as follows:

--Second-order moments provide the capability of spatially profiling the hydrophobicity distribution of amino acid residues. Profiling the distribution of hydrophobicity requires the choice of a profiling shape. Proteins come with all sorts of overall shapes. To profile, ~~on~~ one must choose a particular reference point (the centroid), an appropriate coordinate system (the principal axes of geometry) and a shape representative of the protein (such as an ellipsoidal shape for a globular protein). A representation that is the simplest generalization of the shape of a globular protein is an ellipsoidal representation. This representation can be generated from the molecular moments-of-geometry, i.e., moments-of-inertia for which all amino acid residue centroids are weighted by unity instead of by residue mass. The moments of geometry are obtained as eigenvalues of the following moment-of-geometry matrix written in dyadic notation:

$$\tilde{M}_2 = \sum_i (\tilde{I} |\vec{r}_i - \vec{r}_c|^2 - (\vec{r}_i - \vec{r}_c)(\vec{r}_i - \vec{r}_c)), \quad (\text{Eq. 7})$$

where \tilde{I} is the unit dyadic. The calculation is performed with the centroid (determined by using the amino acid centroids) of the protein as origin. The moments-of-geometry are designated g_1 , g_2 , and g_3 , with $g_1 < g_2 < g_3$. The ellipsoidal representation generated by these moments is written as:

$$x^2 + g_2' y^2 + g_3' z^2 = d^2 \quad (\text{Eq. 8})$$

with $g_2' = g_2/g_1$ and $g_3' = g_3/g_1$. The coordinates, x, y, z , are written in the frame of the principal-geometric-axes. Equation 8 determines a surface (step 135) that can be used to profile the moments of the hydrophobicity distribution.--